

2) choose the most appropriate conditions for the chemical potential realization of the large macromolecules reactive sites, such as proteins and polysaccharides;

3) carry out diagnostics of different binding centers on the possibility of the chemical, van der Waals interaction, hydration and mass transfer processes without costly investment into the experimental part;

4) obtain a general idea of the nutritional components and water role in the food compositions under consideration, for subsequent recommendations of chemical and physicochemical processes stabilization, associated with quality and safety indicators.

This article discusses systems based on sodium alginate (with an increased content of guluronate residues) and pectin (low esterified amidated) with realization of calcium ions chemical potential in various interaction with the remainders of uronic acids.

Calcium, as the most promising binding agent, and under consideration uronate polysaccharides, as widely used substances for obtaining gel-like systems with valuable food properties and technological characteristics, form firmly bound structures in food systems. These structures allow stabilizing the processes of moisture mass transfer and keep it to 30% when passing from the phase of the hydrogel to the xerogel [1].

Nowadays significant relevance is the study of polysaccharide compositions based on sodium alginate and pectin with other polysaccharides. For example, the authors [2] monitored the adsorption properties of the sodium alginate matrix with the participation of guar gum. The article [3] describes the molecular mechanism of lysozyme adsorption to a chemically modified alginate-guar matrix. New biodegradable and antibacterial edible films based on alginate hydrochloride and biguanidine chitosan are described in the article [4]. In the materials of the scientific publication [5] describe microgel of silylated (hydroxypropyl) methyl cellulose, which is considered as a multimodal system for the joint encapsulation of drugs. A group of scientists received alginate fibers coated with chitosan and described their antibacterial effect. [6].

The most obvious advantages are mixed pectin-alginate gels, structured by calcium ions [7, 8].

However, it should be noted, that systems based on this composition remain poorly researched, although they have a significant economic effect when used in various technologies [9-12].

Objects

The purpose of this work is the detailed elaboration of theoretical study the features of molecular complexes equilibrium structures, which are

implemented in the system «uronate polysaccharides – Ca^{2+} » by means of *ab initio* quantum chemistry methods.

Statement of the main material

Quantum chemical modeling is the method of obtaining the molecule electron energy and its wave function, which does not depend on the size and structure of the macromolecule.

It must be borne in mind three determining factors before the construction of a quantum chemical model. Namely, to select the components of the mathematical model, carry out a decision procedure and choose an atomic basis. Thus, to determine the method of obtaining the electron energy and the wave function [13].

The wave function is meant density matrix in density functional theory. It should be noted that this method does not describe any particular chemical system and can be applied to a molecule of any size and to any molecular structure and to any type of chemical binding. [14, 15].

Quantum-chemical models CaGal_4 , CaGul_4 , $\text{CaGul}_2\text{Gal}_2$, presented on the Figure 1 a-c were obtained on the basis of this.

Named images confirm the uniqueness of the Schrödinger equation solution for a given nuclei configuration, electron and spin states of the molecule. This solution is as close as possible to the objects under study, in particular, alginate-pectin-calcium complexes. Beside this, the presented models are applicable to a larger system, taking into account random molecular structures also.

The presented models require elaboration. Semi-empirical calculation methods were used for this. It is most expedient to continue calculations by the method M062x. It is necessary that several additional principles are fulfilled:

1. The results obtained for a system consisting of a minimum molecules set at an infinite distance from each other must correspond to the sum of the results obtained for isolated molecules of this system.

2. Energy, determined by this method, is the upper limit of the electron equation exact solution. The refinements, which were carried out by semi-empirical methods, made it possible to obtain smaller values of the energy than the obtained by molecular mechanic methods models.

Geometric parameters of chelate complexes «uronate polysaccharides – Ca^{2+} » that isolated from Z-matrices for optimized molecules of CaGal_4 , CaGul_4 , $\text{CaGul}_2\text{Gal}_2$ given in Table 1. Subsequently, using the theory of the density functional in the approximation B3LYP with the following modifications: M06, M062X, peculiarities the conformational transformations of uronate polysaccharides complexes with calcium were studied.

The lengths of bonds, torsion angles and valence angles were considered as geometric parameters.

Concerning the construction of macromolecular structures, in particular uronate polysaccharides, it is

fair to say, that in Table 1 the characteristics of the complexes are visually represented: the lengths of the calcium ion with polysaccharides coordination bonds, torsion and valence angles.

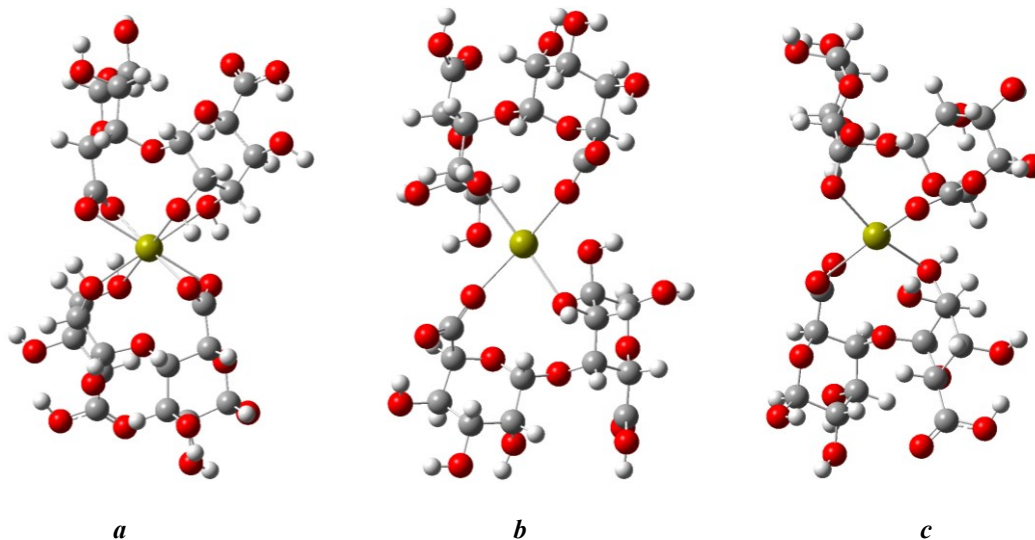


Fig. 1 – Models of stable calcium-uronate systems: a – tetrahyuronate calcium (CaGul₄); b – tetragalacturonate calcium (CaGal₄); c – digalacturonotadigalacturonate calcium (CaGul₂Gal₂)

Table 1 – Geometric parameters of the system «uronate polysaccharides – Ca²⁺ chelate complexes»

| | | Complex | | | | | | | | | | | |
|---|--|--------------------|---------|-------------|-----------|--------------------|----------|-------------------------------------|------------|-------|--|-----------|--|
| | | CaGul ₄ | | | | CaGal ₄ | | CaGul ₂ Gal ₂ | | | | | |
| | | n | d | n | d | n | d | n | d | | | | |
| Length of bond Ca-O _n , Å | | 12 | 2.54038 | 53 | 2.54156 | 30 | 2.46918 | 38 | 2.53946 | | | | |
| | | 78 | 2.52733 | 37 | 2.52801 | 12 | 2.42611 | 8 | 2.49132 | | | | |
| | | 79 | 2.49019 | 38 | 2.49077 | 72 | 2.46897 | 55 | 2.48009 | | | | |
| | | 49 | 2.48383 | 8 | 2.48322 | 54 | 2.42532 | 75 | 2.43800 | | | | |
| | | W-X-Y-Z | | W-X-Y-Z | | W-X-Y-Z | | | | | | | |
| Torsion angles H _w – C _x – O _y – C _z , ° | | φ | | 76-65-50-43 | -61.15840 | 36-26-13-2 | 46.61303 | 79-69-56-45 | -101.31086 | | | | |
| | | ψ | | 35-24-9-2 | -61.15783 | 78-68-55-44 | 46.63952 | 35-24-9-2 | -52.91515 | | | | |
| | | φ | | 52-43-50-65 | 22.59891 | 1-2-13-26 | 20.04796 | 44-45-56-69 | -6.15302 | | | | |
| | | ψ | | 11-2-9-24 | 22.59878 | 43-44-55-68 | 19.94151 | 11-2-9-24 | 15.11548 | | | | |
| Valence angles O _n – Ca – O _m , ° | | n-m | | n-m | | n-m | | | | | | | |
| | | 12-37 | | 114.60009 | | 12-30 | | 76.79737 | | 75-55 | | 76.07383 | |
| | | 8-38 | | 115.46188 | | 72-54 | | 76.77659 | | 38-8 | | 106.73409 | |
| | | 78-53 | | 114.58527 | | - | | - | | - | | - | |
| | | 79-49 | | 115.44966 | | - | | - | | - | | - | |
| | | 49-38 | | 94.79095 | | 72-12 | | 99.95322 | | 75-38 | | 85.60411 | |
| | | 54-37 | | 92.60015 | | 54-30 | | 99.70507 | | 55-8 | | 99.93691 | |
| | | 78-12 | | 92.63874 | | - | | - | | - | | - | |
| 79-8 | | 94.79806 | | - | | - | | - | | - | | | |

Results and discussion

In the model of the complex CaGul_4 all links are equal with a small deviation within the permissible error $2,54038 \pm 0,05716 \text{ \AA}$.

Considering the model of the system CaGal_4 , the values of the calcium bonds lengths with the oxygen atoms of the nearby carboxyl and hydroxyl groups have found a similar tendency. An average value of the bond length is $2,51283 \text{ \AA}$ with permissible deviations within $\pm 0,04386 \text{ \AA}$. Comparing these indicators during the examination of the complex $\text{CaGul}_2\text{Gal}_2$, the average value of the bond length is somewhat smaller. This may indicate greater homogeneity and lower voltage of the binding atoms and more stable position. Thus, the average value of the bond length within the permissible error is $2,43800 \pm 0,04386 \text{ \AA}$.

Estimating the value of the bond length between the residues of uronic acids of polysaccharides with calcium in the complex $\text{CaGul}_2\text{Gal}_2$, it can be noticed, that these values for alginate and pectin have shifted towards the averaging. This is absolutely correct and natural as a result of the binding energies distribution in the system.

Torsion angles of the glycosidic bond were taken (as example of the system $\text{CaGul}_2\text{Gal}_2$) angle φ for atoms $\text{H}_{76}-\text{C}_{65}-\text{O}_{50}-\text{C}_{43}$ and angle ψ for atoms $\text{H}_{52}-\text{C}_{43}-\text{O}_{50}-\text{C}_{65}$ with quantitative characteristics - $101,31086$ and - $6,15302 \text{ \AA}$ respectively (Fig. 2). It is worth noting, that torsion angles for chains of different polysaccharides are very different from each other and the difference is $48,39571$ and $21,2685 \text{ \AA}$.

At the same time in the systems CaGal_4 and CaGul_4 , torsion angles φ and ψ have very similar meanings: $46,62623 \pm 0,0132 \text{ \AA}$ and $-61,158115 \pm 0,00028 \text{ \AA}$ respectively.

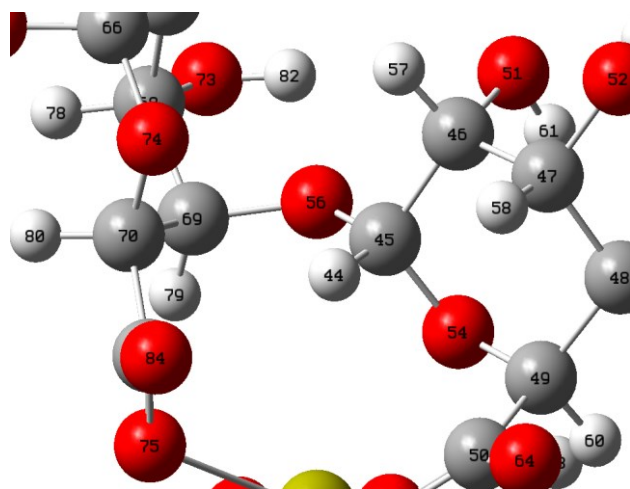


Fig. 2 – Fragment of the model $\text{CaGul}_2\text{Gal}_2$ with the notation of torsion angles φ and ψ ($\text{H}_w-\text{C}_x-\text{O}_y-\text{C}_z$)

Significant differences in torsion and valence angles in the system model $\text{CaGul}_2\text{Gal}_2$ connected with the geometry of uronate polysaccharides dimers. Guluronate remains have a more spatial structure, but galacturonate are more linear. In both structures ionotropic gel formation with the calcium ions participation proceeds successfully, as in the case of homogeneous uronate systems (alginate or pectinic).

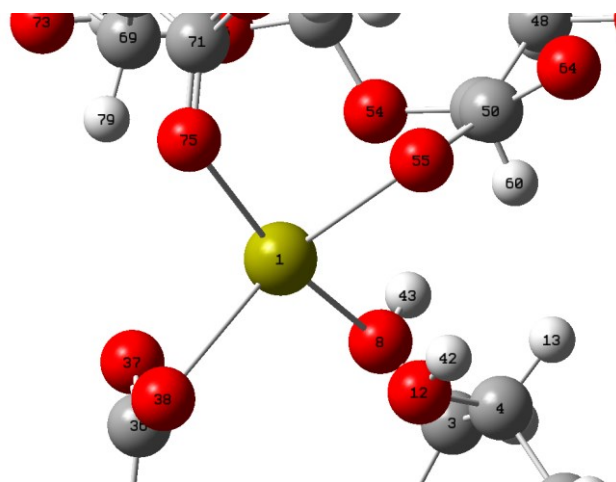


Fig. 3 – Fragment of the model $\text{CaGul}_2\text{Gal}_2$ with the notation of valence angles $\text{O}_n-\text{Ca}-\text{O}_m$

The valence angle with Ca, formed in the field of one uronate polysaccharide and various, given on Fig. 3 (as example of the angle $\text{O}_{79}-\text{Ca}-\text{O}_{49}$ and angle $\text{O}_{79}-\text{Ca}-\text{O}_{12}$).

Conclusions

It is of fundamental importance for understanding the chemistry of the ionotropic gel formation in systems of such polysaccharides, as low esterified amidated pectin and high-guluronate sodium alginate and their compositions, are the spatial arrangement of the set of atoms in these systems; the magnitude and location of bond lengths; values of torsion and valence angles. All of this in a case allows estimating the chemical activity of fragments macromolecules structures in the case of the ionotropic gel formation. This makes it possible to predict the amount of out-bound water, to calculate the optimum proportions of substances for the rational food recipes.

The fact of the ionotropic gel formation in a combined system “alginate-pectin-Ca” was established based on the obtained models and their geometric characteristics.

Chelate complex $\text{CaGul}_2\text{Gal}_2$, which formed, stable during storage, more plastic, softer as opposed to CaGul_4 and stronger than CaGal_4 .

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АНОТАЦІЯ Проведено квантово-хімічне моделювання процесу іонотропного гелеутворення в системах уронатних полісахаридів (альгіната натрія високогулуронатного і пектина низькоетерифікованого амідованого) з кальцієм. Розрахунок взаємодії активних функціональних груп уронатних полісахаридів з іоном кальцію пояснює можливість протікання даного процесу з утворенням наступних хелатних комплексів: кальцій-гулуронатного (CaGul₄), кальцій-галактуронатного (CaGal₄) та кальцій-гулуронат-галактуронатного (CaGal₂Gul₂).

У статті повідомляється про те, що процес взаємодії здійснюється за рахунок хімічного зв'язування карбоксильних та гідроксильних груп уронатних полісахаридів з іоном металу. Встановлено, що кальцій-гулуронатний комплекс має вісім точок зв'язування з іоном кальцію, а комплекси кальцій-галактуронатний та кальцій-гулуронат-галактуронатний – по чотири. Описані довжини зв'язків, величини торсійних кутів та кутів O_n-Ca-O_m в одержаних хелатних комплексах.

Ключові слова: альгінат; пектин; комплексоутворення; квантово-хімічне моделювання.

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